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Towards the Chiral Regime of Lattice QCD

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Maximally Twisted Mass Fermions: Towards the Chiral Regime of Lattice QCD

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We describe results from large scale lattice simulations employing maximally twisted mass fermions. With this approach to lattice QCD small values of the quark mass can be reached which allow for a safe contact with chiral perturbation theory. We show that very precise values for the low energy constants of the effective chiral Lagrangian can be obtained in this way.

1 Introduction

The theory to describe the strong interactions, which is responsible e.g. for the existence of the proton and the neutron, is Quantum Chromodynamics. It postulates the existence of fundamental particles, quarks and gluons, which bind together to form the observed hadron spectrum.

The main problems with QCD are first that the fundamental building blocks, the quarks and gluons, cannot be observed themselves, a phenomenon that is called confinement. Secondly, the binding energy of the hadrons is so large that any perturbative treatment of describing them must fail.

A conceptually very attracting way to study QCD is by means of numerical simulations. To this end, the theory is formulated on a discrete space-time lattice with a certain lattice spacing a. Then the system can essentially be regarded as a statistical physics model and the techniques from statistical mechanics can be employed. Indeed, considering simpler models than QCD, this approach to address quantum field theories has been very successful. However, the application to lattice QCD has turned out to be extremely demanding and in the past a number of approximations had to be made to tackle the problem.

This situation has changed in the last two years dramatically. New algorithms have been developed that allow an order of magnitude faster simulations and modern supercomputer architectures are available now that can reach tens and hundreds of teraflops, such as the one installed at NIC. In this drastically improved situation, it is now possible to really perform realistic lattice QCD simulations, leaving all approximations behind and treating the complete theory.

An important aspect is that the results of such simulations which are obtained at non-vanishing values of the lattice spacing have to be extrapolated to the continuum limit at zero lattice spacing. The original formulation of lattice QCD by K. Wilson[1] has discretization effects that are linear in the lattice spacing. This fact has turned out in practical simulations to be rather problematic since it leads to a slow convergence to the continuum limit.

However, it has been possible to develop alternative formulations of lattice QCD where the effects that are linear in the lattice spacing are completely canceled – we speak of $\mathcal{O}(a)$-improvement – and consequently, the continuum limit can be reached much faster. In this report, we will address one of these approaches, the so-called twisted mass formulation[2,3]. It has to be stressed that there are alternative approaches such as clover improved Wilson fermions and chiral invariant overlap and chirally improved hypercube or truncated perfect action fermions, see e.g. ref.[4] for a discussion and references to these different kind of lattice actions. It is important that different lattice fermions are used in lattice QCD since they have different kind of systematic errors. Using different lattice discretizations of QCD and performing a corresponding continuum limit provides a most valuable test of physical results that come from lattice QCD.

The results that are shown here were obtained within a large European Twisted Mass Collaboration (ETMC) which comprises a number of different places in Europe, i.e. Cyprus: Univ. of Nikosia; France: Univ. of Paris Sud and LPSC Grenoble; Germany: Humboldt Univ. zu Berlin, Univ. of Münster, DESY in Hamburg and Zeuthen; Great Britain: Univ. of Glasgow and Liverpool, Italy Univ. of Rome I, II and III, ECT* Trento; Netherlands: Univ. of Groningen; Spain: Univ. of Valencia; Switzerland: Univ. Zürich. This collaboration brings together a large amount of different expertise, ranging from code optimization and algorithm development to physical applications that are directly relevant for ongoing experiments and phenomenological analyses. A first account of our results can be found in ref.[5]. Overviews can be found in[6,7].

2 Choice of Lattice Action

What we will consider in this contribution is the Wilson twisted mass fermionic lattice action for two flavours of degenerate quarks which reads (in the so called twisted basis[2] and fermion fields with continuum dimensions)

$$\begin{aligned} S_{\rm tm} = a^4 \sum_x \Big\{ \bar\chi_x \left[m_0 + i\gamma_5\tau_3\mu + \frac{4r}{a} \right] \chi_x \\ + \frac{1}{2a} \sum_{\nu=1}^{4} \bar\chi_x \left[U_{x,\nu}(-r+\gamma_\nu)\chi_{x+\hat\nu} + U^\dagger_{x-\hat\nu,\nu}(-r-\gamma_\nu)\chi_{x-\hat\nu} \right] \Big\} . \end{aligned} \tag{1}$$

Here am_0 is the bare untwisted quark mass and $a\mu$ the bare twisted mass, τ_3 is the third Pauli matrix acting in flavour space and r is the Wilson parameter, which we set to one in our simulations. Twisted mass fermions are said to be at *maximal twist* if the bare untwisted mass is tuned to its critical value, $m_{\rm crit}$. We will discuss later how this can be achieved in practice.

In the gauge sector we use the so called tree-level Symanzik improved gauge action (tlSym)[8], which includes besides the plaquette term $U^{1\times1}_{x,\mu,\nu}$ also rectangular (1×2) Wilson loops $U^{1\times2}_{x,\mu,\nu}$

$$S_g = \frac{\beta}{3} \sum_x \left(b_0 \sum_{\substack{\mu,\nu=1 \\ 1\le\mu<\nu}}^{4} \{1 - {\rm Re\,Tr}(U^{1\times1}_{x,\mu,\nu})\} + b_1 \sum_{\substack{\mu,\nu=1 \\ \mu\neq\nu}}^{4} \{1 - {\rm Re\,Tr}(U^{1\times2}_{x,\mu,\nu})\} \right) \tag{2}$$

with β the bare inverse coupling, $b_1 = -1/12$ and the (proper) normalisation condition $b_0 = 1 - 8b_1$. Note that at $b_1 = 0$ this action becomes the usual Wilson plaquette gauge action.

2.1 $\mathcal{O}(a)$ Improvement

As mentioned before, $\mathcal{O}(a)$ improvement can be obtained by tuning Wilson twisted mass fermions to maximal twist. In fact, it was first proved in Ref.[3] that parity even (and therefore physical) correlators are free from $\mathcal{O}(a)$ lattice artifacts at maximal twist by using spurionic symmetries of the lattice action. Later on it was realised[9,10] that a simpler proof is possible based on the parity symmetry of the continuum QCD action and the use of the Symanzik effective theory.

From this latter way of proving $\mathcal{O}(a)$ improvement, it becomes also clear how to define maximal twist: first, choose an operator odd under parity (in the physical basis) which has a zero expectation value in the continuum. Second, at a non-vanishing value of the lattice spacing tune the expectation value of this operator to zero by adjusting the value of am_0. This procedure, which has been proposed in[11,12] and has been theoretically analysed in[9], is sufficient to define maximal twist independently of the chosen operator. To approach smoothly the continuum limit this tuning has to be performed at fixed physical situation while decreasing the lattice spacing.

Besides being a theoretically sound formulation of lattice QCD, Wilson twisted mass fermions offer a number of advantages when tuned to maximal twist: (i) in this case automatic $\mathcal{O}(a)$ improvement is obtained by tuning only one parameter, the bare untwisted quark mass, while avoiding additional tuning of operator-specific improvement-coefficients; (ii) the mixing pattern in the renormalisation process can be significantly simplified; (iii) the twisted mass provides an infra-red regulator helping to overcome possible problems with ergodicity in molecular dynamics based algorithms.

The main drawback of the twisted mass approach is the explicit breaking of parity and isospin symmetry which are only restored when the continuum limit is reached. However, due to $\mathcal{O}(a)$ improvement, this breaking is an $\mathcal{O}(a^2)$ effect as confirmed by simulations performed in the quenched approximation[13,14]. Furthermore, theoretical considerations indicate that these $\mathcal{O}(a^2)$ effects may become large *only* for the particular case of the neutral pion mass[15]. This expectation is confirmed by results from numerical simulations for other quantities considered so far.

The condition of tuning the parameters of the theory such that a parity odd operator vanishes can be reformulated as the condition that the so-called PCAC mass is tuned to zero. Here the PCAC mass

$$m_{\mathrm{PCAC}} = \frac{\sum_{\mathbf{x}} \langle \partial_0 A_0^a(x) P^a(0) \rangle}{2 \sum_{\mathbf{x}} \langle P^a(x) P^a(0) \rangle}\,, \qquad a = 1, 2 \tag{3}$$

is evaluated at large enough time separation, such that the pion ground state is dominant.

The strategy we have followed is to take the value of am_{crit} from the simulation at the lowest available value $a\mu_{\mathrm{min}} \ll a\Lambda_{\mathrm{QCD}}$. In this situation $\mathcal{O}(a)$ improvement is still guaranteed, because working at μ_{min} merely leads to $\mathcal{O}(a\mu_{\mathrm{min}}\Lambda_{\mathrm{QCD}})$ effects in m_{crit} and $\mathcal{O}(a^2\mu_{\mathrm{min}}\Lambda_{\mathrm{QCD}})$ relative corrections in physical quantities[9]. Although these theoretical arguments show that we are left with only $\mathrm{O}(a^2)$ lattice artefacts, numerical computations are required to determine the coefficient multiplying the a^2-term for the observables of interest. In our simulations the condition of maximal twist has been numerically realised with good accuracy, which in this context means $m_{\mathrm{PCAC}}(\mu_{\mathrm{min}})/\mu_{\mathrm{min}} < a\Lambda_{QCD}$ within statistical errors ($a\Lambda_{QCD} \sim 0.1$ in our case).

The algorithm we used is a HMC algorithm with mass preconditioning[16,17] and multiple time scale integration described in detail in Ref.[18]. The trajectory length τ was set to $\tau = 1/2$ in all our runs. While the plaquette autocorrelation times are typically O(10-50), for quantities such as $am_{\rm PS}$ or $af_{\rm PS}$ we find them to be substantially smaller, typically by a factor of 5-10.

2.2 $f_{\rm PS}$ and $m_{\rm PS}$ As a Function of the Quark Mass

The *charged* pseudo scalar meson mass $am_{\rm PS}$ is as usual extracted from the time exponential decay of appropriate correlation functions. In contrast to pure Wilson fermions, for maximally twisted mass fermions an exact lattice Ward identity allows to extract the (charged) pseudo scalar meson decay constant $f_{\rm PS}$ with no need to compute any renormalisation constant since $Z_P = 1/{Z_\mu}^2$.

In our χPT based analysis, we take into account finite size corrections because on our lattices at the lowest and next-to-lowest μ-values they turn out to affect $am_{\rm PS}$ and, in particular, $af_{\rm PS}$ in a significant way. We have used continuum χPT to describe consistently the dependence of the data both on the finite spatial size (L) and on μ.

We fit the appropriate ($N_f = 2$) χPT formulae[19,20]

$$m_{\rm PS}^2(L) = 2B_0\mu\left[1+\frac{1}{2}\xi\tilde{g}_1(\lambda)\right]^2\left[1+\xi\log(2B_0\mu/\Lambda_3^2)\right]\,, \tag{4}$$

$$f_{\rm PS}(L) = F\left[1-2\xi\tilde{g}_1(\lambda)\right]\left[1-2\xi\log(2B_0\mu/\Lambda_4^2)\right]\,, \tag{5}$$

to our raw data for $m_{\rm PS}$ and $f_{\rm PS}$ simultaneously. Here

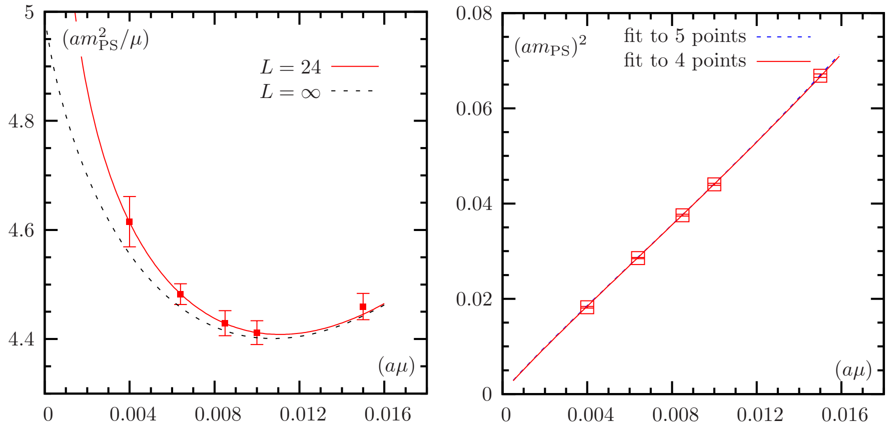
$$\xi = 2B_0\mu/(4\pi F)^2\,, \qquad \lambda = \sqrt{2B_0\mu L^2}\,. \tag{6}$$

The finite size correction function $\tilde{g}_1(\lambda)$ was first computed by Gasser and Leutwyler in Ref.[19] and is also discussed in Ref.[20] from which we take our notation (except that our normalisation of f_π is 130.7 MeV). In Eqs. (4) and (5) NNLO χPT corrections are assumed to be negligible. The formulae above depend on four unknown parameters, B_0, F, Λ_3 and Λ_4, which will be determined by the fit. For $\mu = 0.004$ and $\mu = 0.0064$ we found the effect of finite size corrections to be 0.5% and 0.2% for the pseudo scalar mass and 2.2% and 0.9% for the pseudo scalar decay constant, respectively. For our larger values of μ the finite size corrections are negligible.

We determine $a\mu_\pi$, the value of $a\mu$ at which the pion assumes its physical mass, by requiring that the ratio $[\sqrt{[m_{\rm PS}^2(L=\infty)]}/f_{\rm PS}(L=\infty)]$ takes the value $(139.6/130.7) = 1.068$. From the knowledge of $a\mu_\pi$ we can evaluate $\bar{l}_{3,4} \equiv \log(\Lambda_{3,4}^2/m_\pi^2)$ and using f_π the value of the lattice spacing a in fm.

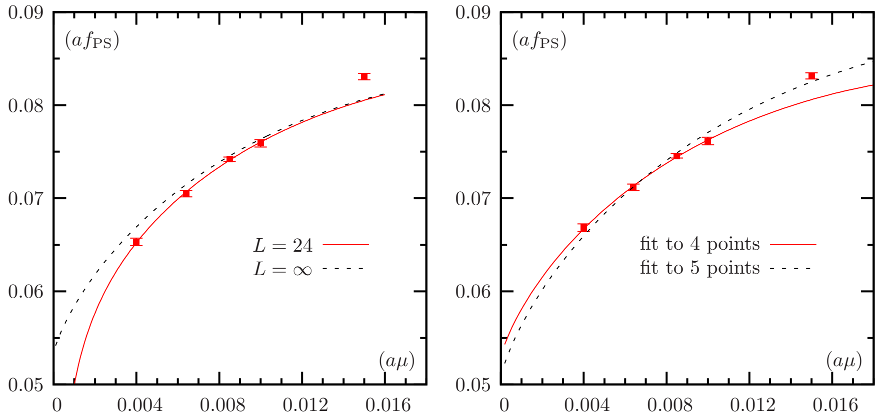
For our lightest four μ-values, we find an excellent fit to our data on $f_{\rm PS}$ and $m_{\rm PS}$ (see figures 1 and 2). The fitted values of the four parameters are

$$\begin{aligned} 2aB_0 &= 4.99(6)\,, \\ aF &= 0.0534(6)\,, \\ \log(a^2\Lambda_3^2) &= -1.93(10)\,, \\ \log(a^2\Lambda_4^2) &= -1.06(4)\,. \end{aligned} \tag{7}$$



(a) (b)

Figure 1. In (a) we show $(am_{\rm PS})^2/(a\mu)$ as a function of $a\mu$. We plot the χPT fit of Eq. (4) applied to the raw data on the $L = 24$ lattice from the lowest four μ-values. We represent the finite size correction by the dashed line. In (b) we show $(am_{\rm PS})^2$ as a function of $a\mu$. Here we present two χPT fits with Eq. (4), one taking all data points and one leaving out the point at the largest value $a\mu = 0.015$. Also in figure (b) we show the $L = 24$ data points.



(a) (b)

Figure 2. We show $af_{\rm PS}$ as a function of $a\mu$ together with fits to χPT formula Eq. (5). In (a) we show the fit applied to the raw data on the $L = 24$ lattice at the 4 lowest values of $a\mu$. We represent the finite size correction by the dashed curve. In (b) we present two fits, one taking all data and one leaving out the point at the largest value $a\mu = 0.015$. Here we show only the finite size corrected ($L \to \infty$) data points.

Our data are clearly sensitive to Λ_3 as visualised in figure 1(a). We obtain

$$a\mu_\pi = 0.00078(2), \qquad \bar{l}_3 = 3.65(12), \qquad \bar{l}_4 = 4.52(06) \tag{8}$$

which compares nicely with other determinations (for a review see Ref.[21]).

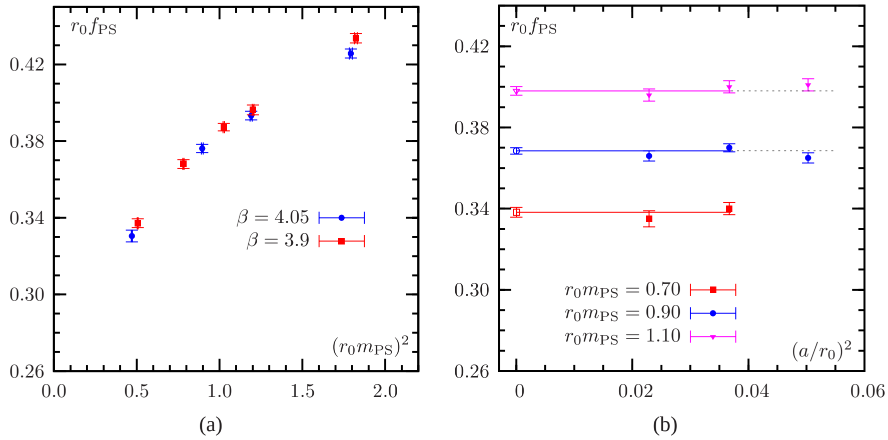


Figure 3. (a) $r_0 f_{\rm PS}$ as a function of $(r_0 m_{\rm PS})^2$ for $\beta = 3.9$ and $\beta = 4.05$. (b) Continuum extrapolation of $f_{\rm PS}$ at fixed volume for three reference values of $r_0 m_{\rm PS}$. The data points at $\beta = 3.8$ are not used.

3 Summary

In this contribution we have presented results of simulations of lattice QCD with $N_f = 2$ maximally twisted Wilson quarks. We reached a pseudo scalar meson mass of about $300\ \mathrm{MeV}$. The numerical stability and smoothness of the simulations allowed us to obtain precise results for the pseudo scalar mass and decay constant which in turn led to determine the low energy constants of the effective chiral Lagrangian. In particular, we find for the pseudo scalar decay constant in the chiral limit $F = 121.3(7)\ \mathrm{MeV}$, and $\bar{l}_3 = 3.65(12)$ and $\bar{l}_4 = 4.52(6)$ where only statistical errors are given. Our results at the two values of the lattice spacing which are used for a continuum extrapolation show almost negligible lattice spacing artefacts which can be seen from fig. 3, see also refs.[7,22], where we show the results for the pseudo scalar decay constant. In the left panel, we exhibit $r_0 f_{\rm PS}$ for two values of the lattice spacing demonstrating that the data scale very nicely. In the right panel we show $r_0 f_{\rm PS}$ at fixed values of the pseudo scalar mass, $r_0 m_{\rm PS}$. In this figure we also show results for an additional value of the lattice spacing which is, however, not used for a continuum extrapolation since it is presently not clear whether our physical condition to reach maximal twist is realized here.

Besides the here described determination of the low energy constants, our collaboration is also computing many more physical observables from the existing configurations from maximally twisted mass fermions. These are the full octet and decuplet spectra[23], moments of parton distribution functions[24], non-perturbatively obtained renormalization constants using the RI-MON scheme[25], light quark masses and decay constants[26,27], charm physics[28], meson form factors[29], exploration of the ϵ-regime of chiral perturbation theory[30], study of cut-off effects at tree-level of perturbation theory[31], neutral mesons[32], overlap fermions on twisted mass sea quarks[33,34] and twisted mass fermions at non-vanishing temperature[35].

All these results obtained from maximally twisted mass fermions and two mass degenerated flavours of quarks are very encouraging and promising. They suggest that indeed maximally twisted mass fermions provide a very valuable formulation of lattice QCD. It is therefore most natural to extend the present study by incorporating the strange and the charm quarks as dynamical degrees in the simulation. This is possible using the setup of ref.[36] and has already been explored in ref.[37]. The simulations for this realistic setup of QCD are presently ongoing and the tuning to maximal twist is already well advanced. Thus, it is to be expected that similar precise results for many physical quantities can be obtained in the near future.

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